

Request Noble Jarrell Access DB# 150213 14  
SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabika Doss Examiner #: 7414 Date: 4/7/05  
Art Unit: 1616 Phone Number 20622 Serial Number: 10/350,532  
Mail Box and Bldg/Rm Location: 4C70, Rm, 4A45 Results Format Preferred (circle): PAPER DISK E-MAIL  
(S11C)

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention: Process of Prep. of 1-[3-dimethylaminopropyl]-1-(4-  
Inventors (please provide full names): Rajamannar et al. Thorophant, S. et al.

Earliest Priority Filing Date: 321 of PCT / Int. 03 / 600006. 1/7/03

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for the process of making  
iso-benzofuran of formula 1 as in cl 1, 4, 41.

Please attached sheet

Thank you

STAFF USE ONLY		Type of Search	Vendors and cost where applicable
Searcher:	<u>Noble</u>	NA Sequence (#)	STN <u>1146</u>
Searcher Phone #:		AA Sequence (#)	Dialog
Searcher Location:		Structure (#)	Questel/Orbit
Date Searcher Picked Up:	<u>4/11/05</u>	Bibliographic	Dr.Link
Date Compiled	<u>4/11/05</u>	Litigation	Lexis/Nexis
Searcher Prep. Review Time	<u>15</u>	Patent	Sequence Systems
Clerical Prep. Time:		Patent Faculty	WWW/Internet
Review Time	<u>73</u>	Other	Other (specify)

=> d his

(FILE 'HOME' ENTERED AT 09:52:34 ON 11 APR 2005)

FILE 'HCAPLUS' ENTERED AT 09:53:38 ON 11 APR 2005

L1 1 US20050043550/PN  
E IN2002-847/AP, PRN  
E IN2002-MUM847/AP, PRN

L2 FILE 'WPIX' ENTERED AT 09:59:09 ON 11 APR 2005  
1 US20050043550/PN

L3 FILE 'HCAPLUS' ENTERED AT 10:00:08 ON 11 APR 2005  
1 (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10 OR W02004-IN6)/AP, P  
L4 1 L1 OR L3

FILE 'REGISTRY' ENTERED AT 10:01:11 ON 11 APR 2005

L5 FILE 'HCAPLUS' ENTERED AT 10:01:14 ON 11 APR 2005  
TRA L4 1- RN : 28 TERMS

L6 FILE 'REGISTRY' ENTERED AT 10:01:15 ON 11 APR 2005  
28 SEA L5

L7 FILE 'WPIX' ENTERED AT 10:01:19 ON 11 APR 2005  
1 (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10 OR W02004-IN6)/AP, P  
L8 1 L2 OR L7

=> b hcap

FILE 'HCAPLUS' ENTERED AT 10:02:19 ON 11 APR 2005

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FILE COVERS 1907 - 11 Apr 2005 VOL 142 ISS 16  
FILE LAST UPDATED: 10 Apr 2005 (20050410/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all 14 tot

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2003:551309 HCAPLUS  
DN 139:117333  
ED Entered STN: 18 Jul 2003  
TI Process for the preparation of 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile via cyanation of the corresponding chloride or bromide precursors.  
IN Thennati, Rajamannar; Kilaru, Srinivasu; Chinnapillai, Rajendran; Patel, Nileshkumar Sureshbhai  
PA Sun Pharmaceutical Industries Limited, India  
SO PCT Int. Appl., 41 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM A61K  
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

FAN. CNT 1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003057132	A2	20030717	WO 2003-IN6	20030107 <--
	WO 2003057132	A3	20040226		
	WO 2003057132	C1	20040415		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2005043550	A1	20050224	US 2004-500532	20040719 <--
PRAI	IN 2002-MU10	A	20020107		<--
	IN 2002-MU18	A	20020110		<--
	IN 2002-MU847	A	20020930		<--
	WO 2003-IN6	W	20030107		

CLASS  
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2003057132	ICM	A61K	
US 2005043550	ECLA	C07D307/87B	<--
OS	CASREACT	139:117333; MARPAT 139:117333	



I

- AB Title compound (I; R = cyano) (citalopram) was prepared by treatment of I (R = Cl, Br) with a cyanide source in the presence of I<sup>-</sup> in an amide, amine, or polyether solvent followed by treatment of the crude product containing 1-[3-(methylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile and 5-carboxamido-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)phthalide impurities with a phosphorus oxyhalide, phosphorus oxide cyanide reversal agent, and purification using a solvent system comprising a hydrocarbon and alc., ester, ether, ketone, or mixture thereof. Thus, citalopram containing 4.7% amide and 0.72% desmethylcitalopram impurities was heated with POC13 in PhMe at 70° for 1 h. The mixture was poured into water and pH was adjusted to 2.0-2.5 with aqueous HCl. The PhMe layer was separated and the pH of the aqueous layer was adjusted to 9.0-9.5 with aqueous NH3 followed by extraction with PhMe to give product containing 0.05% and 0.23% of the amide and desmethylcitalopram resp.
- ST citalopram prepn purifn phosphorus oxychloride; halodimethylaminopropylfluorophenylidihydroisobenzofuran cyanation
- IT Solvents (halogenated; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Cyanation catalysts (iodide ion; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Iodides, reactions RL: RGT (Reagent); RACT (Reactant or reagent) (metal iodides; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

- IT Cyanation  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Alcohols, uses  
 Amides, uses  
 Amines, uses  
 Aromatic hydrocarbons, uses  
 Esters, uses  
 Ethers, uses  
 Hydrocarbons, uses  
 Ketones, uses  
 Nitriles, uses  
 Nitro compounds  
 Polyethers, uses  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 62498-67-3P 64372-56-1P  
 RL: BYP (Byproduct); PREP (Preparation)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 59729-32-7P, Citalopram hydrobromide 59729-33-8P, 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 60-29-7, Diethyl ether, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 71-23-8, n-Propanol, uses 108-88-3, Toluene, uses 110-82-7, Cyclohexane, uses 110-86-1, Pyridine, uses 141-78-6, Ethyl acetate, uses 142-82-5, n-Heptane, uses 1330-20-7, Xylene, uses 27175-64-0, Lutidine  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 109-54-6, Dimethylaminopropyl chloride 143-33-9, Sodium cyanide 151-50-8, Potassium cyanide 352-13-6, 4-Fluorophenyl magnesium bromide 460-00-4, 4-Fluorobromobenzene 544-92-3, Cuprous cyanide 19070-16-7 64169-34-2, 5-Bromophthalide 64169-39-7 561304-25-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 1314-56-3, Phosphorus pentoxide, reactions 7681-11-0, Potassium iodide, reactions 10025-87-3, Phosphorus oxychloride  
 RL: RGT (Reagent); RACT (Reactant or reagent)  
 (process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)

=> b wpix  
 FILE 'WPIX' ENTERED AT 10:02:46 ON 11 APR 2005  
 COPYRIGHT (C) 2005 THE THOMSON CORPORATION

FILE LAST UPDATED: 6 APR 2005 <20050406/UP>  
 MOST RECENT DERWENT UPDATE: 200522 <200522/DW>  
 DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.  
PLEASE CHECK:  
<http://thomsonderwent.com/support/dwpiref/reftools/classification/code-revision/>  
FOR DETAILS. <<<

=> d all 18 tot

L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN  
AN 2003-636635 [60] WPIX  
DNC C2003-174026  
TI Preparation of citalopram used as antidepressant agent involves reacting corresponding 5-chloro or bromo derivative with cyanide source.  
DC B02  
IN CHINNAPILLAI, R; KILARU, S; PATEL, N S; THENNATI, R; RAJAMANNAR, T;  
RAJENDRAN, C; SRINIVASU, K  
PA (SUNP-N) SUN PHARM IND LTD; (PATE-1) PATEL N S; (RAJA-I) RAJAMANNAR T;  
(RAJE-I) RAJENDRAN C; (SRIN-I) SRINIVASU K  
CYC 102  
PI WO 2003057132 A2 20030717 (200360)\* EN 21 A61K000-00  
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS  
LU MC MW MZ NL OA PT SD SE SI SK SL SZ TR TZ UG ZM ZW  
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK  
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR  
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT  
RO RU SC SD SE SG SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA  
ZM ZW  
AU 2003222435 A1 20030724 (200421) A61K000-00  
US 2005043550 A1 20050224 (200515) C07D307-87 <--  
ADT WO 2003057132 A2 WO 2003-IN6 20030107; AU 2003222435 A1 AU 2003-222435  
20030107; US 2005043550 A1 WO 2003-IN6 20030107, US 2004-500532 20040719  
FDT AU 2003222435 A1 Based on WO 2003057132  
PRAI IN 2002-MU847 20020930; IN 2002-MU10  
20020107; IN 2002-MU18 20020110  
IC ICM A61K000-00; C07D307-87  
AB WO2003057132 A UPAB: 20031030

NOVELTY - Preparation of citalopram (I) comprises:

(a) reacting the corresponding 5-chloro or bromo derivative (II) with a cyanide source in the presence of iodide and a solvent;  
(b) reacting the obtained crude compound with cyanide reversal agent and isolating the base of (I) from the reaction mixture, and  
(c) purifying the base from a solvent system.

DETAILED DESCRIPTION - Preparation of citalopram (I) comprises:  
(a) reaction of a corresponding 5-chloro or bromo derivative of formula (II) with a cyanide source in the presence of iodide and a solvent (S1);

(b) reacting the obtained crude compound (I) with a cyanide reversal agent, isolating the base of (I) from the reaction mixture and optionally converting (I) into a salt followed by conversion into the base of (I), and

(c) purifying the base from a solvent system comprising a first solvent and second solvent.

R = Br or Cl.

The obtained crude product contains desmethylcitalopram impurity comprising 1-(3-(methylamino)propyl)-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofuran carbonitrile and amide impurity comprising 5-carboxamide-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-phthalide. The first solvent is hydrocarbon and the second solvent is alcohol, ester, ether and/or ketone. (S1) Comprises amides, amines or polyethers.

INDEPENDENT CLAIMS are also included for:

(1) preparation of (I) by step (a) per se;  
(2) preparation of (I) by step (b) per se, where the cyanide reversal agent comprises phosphorus oxyhalides or phosphorus oxides, and  
(3) purifying (I) which comprises crystallizing (I) from the solvent system as in step (c).

ACTIVITY - Antidepressant.

No biological data is given.

MECHANISM OF ACTION - None given.

USE - Used as an antidepressant agent (claimed).

ADVANTAGE - High quality (I) is obtained in improved yield by reversing the amide impurity to the desired (I). The process eliminates the use of multiple solvents and operations making it user friendly, and avoids extensive and expensive purification.

Dwg. 0/0

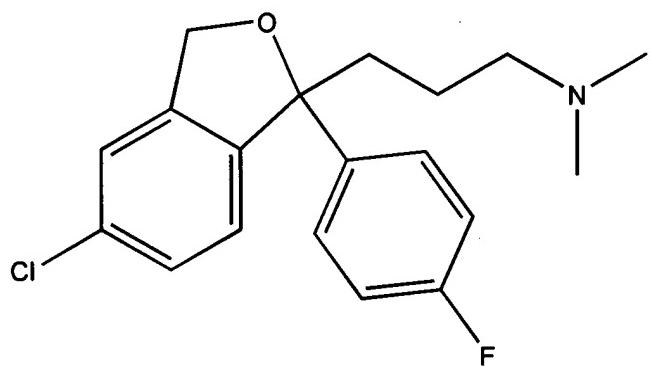
FS CPI

FA AB; GI; DCN

MC CPI: B06-A02; B14-J01A1

=> b home  
FILE 'HOME' ENTERED AT 10:02:55 ON 11 APR 2005

=>



3-(5-chloro-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-1-yl)-*N,N*-dimethylpropan-1-amine

C<sub>19</sub>H<sub>21</sub>ClFNO

=> b reg  
FILE 'REGISTRY' ENTERED AT 13:43:13 ON 11 APR 2005  
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STRUCTURE FILE UPDATES: 10 APR 2005 HIGHEST RN 848184-66-7  
DICTIONARY FILE UPDATES: 10 APR 2005 HIGHEST RN 848184-66-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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\*\*\*\*\*  
\* \*  
\* The CA roles and document type information have been removed from \*  
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\* available and contains the CA role and document type information. \*  
\* \*  
\*\*\*\*\*

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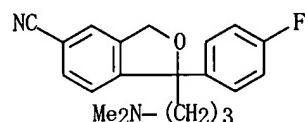
Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide 19 tot

L9 ANSWER 1 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
RN **500733-84-6** REGISTRY  
ED Entered STN: 26 Mar 2003  
CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monoacetate (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Citalopram acetate  
MF C20 H21 F N2 O . C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

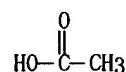
CM 1

CRN 59729-33-8  
CMF C20 H21 F N2 O



CM 2

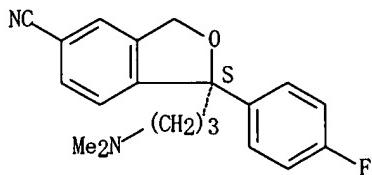
CRN 64-19-7  
CMF C2 H4 O2



2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 2 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **490037-56-4** REGISTRY  
 ED Entered STN: 14 Feb 2003  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, labeled with tritium, (1S)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 IL XH-3

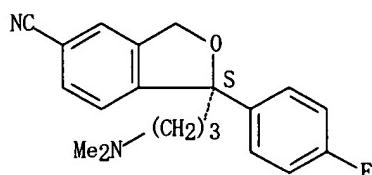
Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 3 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **481047-50-1** REGISTRY  
 ED Entered STN: 24 Jan 2003  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide, (1S)- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN (S)-Citalopram hydrobromide  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O . Br H  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 CRN (128196-01-0)

Absolute stereochemistry. Rotation (+).



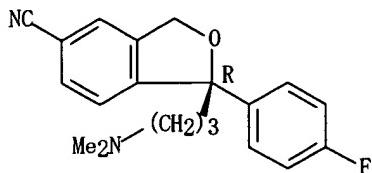
● HBr

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 4 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **481047-49-8** REGISTRY  
 ED Entered STN: 24 Jan 2003  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide, (1R)- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN (R)-Citalopram hydrobromide  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O . Br H

SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 CRN (128196-02-1)

Absolute stereochemistry. Rotation (-).



● HBr

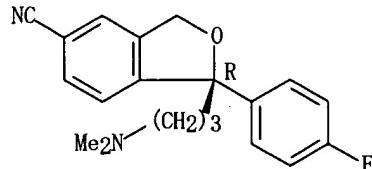
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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 5 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 219861-53-7 REGISTRY  
 ED Entered STN: 21 Feb 1999  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1R)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN R-(-)-Citalopram oxalate  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O . C2 H2 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, RTECS\*, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)

CM 1

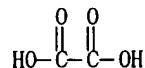
CRN 128196-02-1  
 CMF C20 H21 F N2 O

Absolute stereochemistry. Rotation (-).



CM 2

CRN 144-62-7  
 CMF C2 H2 O4



4 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 6 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 219861-08-2 REGISTRY  
 ED Entered STN: 21 Feb 1999

CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN Cipralex

CN Escitalopram oxalate

CN Lexapro

CN Lu 26-054-0

FS STEREOSEARCH

MF C20 H21 F N2 O . C2 H2 O4

CI COM

SR CA

LC STN Files: ADISINSIGHT, BIOSIS, BIOTECHNO, CA, CAPLUS, CHEMCATS, EMBASE, IMSPATENTS, IMSRESEARCH, IPA, MRCK\*, PATDPASPC, PROUSDDR, PS, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPATFULL

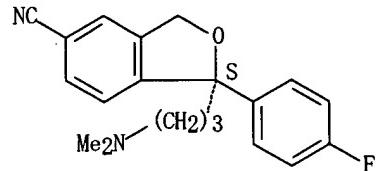
(\*File contains numerically searchable property data)

CM 1

CRN 128196-01-0

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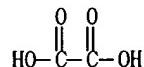
Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7

CMF C2 H2 O4



23 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

23 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 7 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN

RN 207559-01-1 REGISTRY

ED Entered STN: 24 Jun 1998

CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN ( $\pm$ )-Citalopram oxalate

CN Citalopram oxalate

MF C20 H21 F N2 O . C2 H2 O4

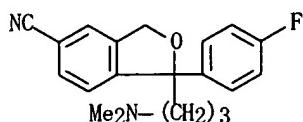
SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

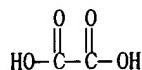
CM 1

CRN 59729-33-8

CMF C20 H21 F N2 O

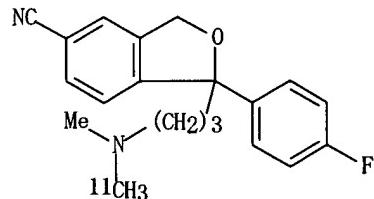


CM 2

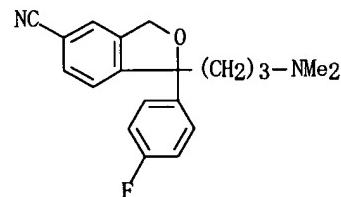
CRN 144-62-7  
CMF C2 H2 O415 REFERENCES IN FILE CA (1907 TO DATE)  
15 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 8 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 141258-68-6 REGISTRY  
 ED Entered STN: 08 May 1992  
 CN 5-Isobenzofuranonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]-, (-) (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O  
 SR CA  
 LC STN Files: CA, CAPLUS

Rotation (-).

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 9 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 135021-05-5 REGISTRY  
 ED Entered STN: 19 Jul 1991  
 CN 5-Isobenzofuranonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, labeled with tritium (9CI) (CA INDEX NAME)  
 MF C20 H21 F N2 O  
 SR CA  
 LC STN Files: CA, CAPLUS  
 IL XH-3

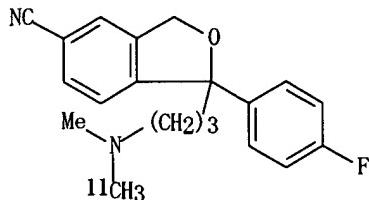


3 REFERENCES IN FILE CA (1907 TO DATE)

## 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

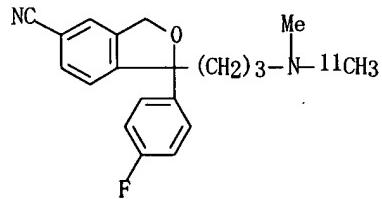
L9 ANSWER 10 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **134915-04-1** REGISTRY  
 ED Entered STN: 19 Jul 1991  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]-, (+)- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O  
 SR CA  
 LC STN Files: CA, CAPLUS

Rotation (+).



3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

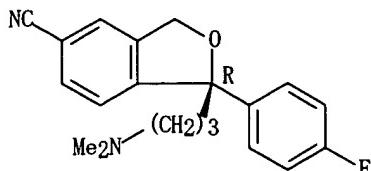
L9 ANSWER 11 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **129356-76-9** REGISTRY  
 ED Entered STN: 14 Sep 1990  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylmethyl-11C-amino)propyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H21 F N2 O  
 SR CA  
 LC STN Files: CA, CAPLUS



3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 12 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **128196-02-1** REGISTRY  
 ED Entered STN: 13 Jul 1990  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1R)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (R)-  
 OTHER NAMES:  
 CN (R)-Citalopram  
 CN R-(-)-Citalopram  
 FS STEREOSEARCH  
 MF C20 H21 F N2 O  
 CI COM  
 SR CA  
 LC STN Files: ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, IMSPATENTS, IMSRESEARCH, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).

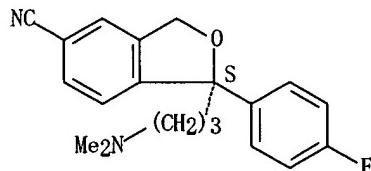


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

46 REFERENCES IN FILE CA (1907 TO DATE)  
46 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 13 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **128196-01-0** REGISTRY  
 ED Entered STN: 13 Jul 1990  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (1S)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (S)-  
 OTHER NAMES:  
 CN (S)-Citalopram  
 CN Escitalopram  
 CN S-(+)-Citalopram  
 FS STEREOSEARCH  
 MF **C20 H21 F N2 O**  
 CI COM  
 SR CA  
 LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MRCK\*, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).



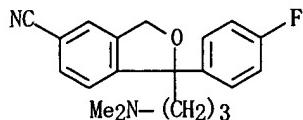
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

136 REFERENCES IN FILE CA (1907 TO DATE)  
136 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 14 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN **107190-73-8** REGISTRY  
 ED Entered STN: 21 Mar 1987  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, (E)-2-butenedioate  
 FS STEREOSEARCH  
 MF **C20 H21 F N2 O . x C4 H4 O4**  
 SR CA  
 LC STN Files: CA, CAPLUS, IMSPATENTS, IMSRESEARCH, PS

CM 1

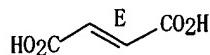
CRN 59729-33-8  
 CMF C20 H21 F N2 O



CM 2

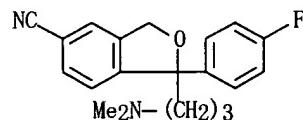
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 15 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 85118-27-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN ( $\pm$ )-Citalopram hydrochloride  
 CN Citalopram hydrochloride  
 DR 316121-47-8  
 MF C20 H21 F N2 O . C1 H  
 CI COM  
 SR European Union (EU)  
 LC STN Files: CA, CAPLUS, CHEMLIST, PS, TOXCENTER, USPAT2, USPATFULL  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 CRN (59729-33-8)



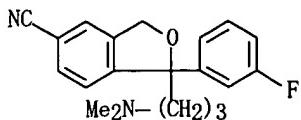
● HCl

13 REFERENCES IN FILE CA (1907 TO DATE)  
 13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 16 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64372-51-6 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(3-fluorophenyl)-1,3-dihydro-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 MF C20 H21 F N2 O . C2 H2 O4  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)

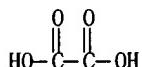
CM 1

CRN 64372-50-5  
 CMF C20 H21 F N2 O



CM 2

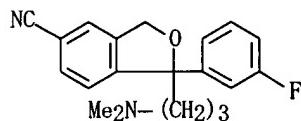
CRN 144-62-7  
 CMF C2 H2 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 17 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64372-50-5 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(3-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H21 F N2 O  
 CI COM  
 LC STN Files: BEILSTEIN\*  
 (\*File contains numerically searchable property data)

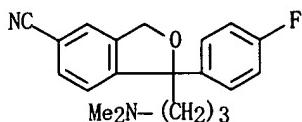


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

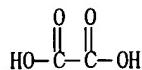
L9 ANSWER 18 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-59-1 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, ethanedioate (9CI) (CA INDEX NAME)  
 MF C20 H21 F N2 O . x C2 H2 O4  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, IMSPATENTS, IMSRESEARCH, USPATFULL

CM 1

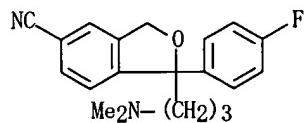
CRN 59729-33-8  
 CMF C20 H21 F N2 O



CM 2

CRN 144-62-7  
CMF C2 H2 O41 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 19 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 59729-33-8 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN ( $\pm$ )-Citalopram  
 CN 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile  
 CN Bonitrile  
 CN Citalopram  
 CN Lu 10-171  
 CN Nitalapram  
 FS 3D CONCORD  
 DR 128196-03-2, 103146-27-6  
 MF C20 H21 F N2 O  
 CI COM  
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOPHARMA, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB\*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK\*, PROMT, PROUSSDR, PS, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*, WHO  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1438 REFERENCES IN FILE CA (1907 TO DATE)  
 11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1443 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 20 OF 20 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 59729-32-7 REGISTRY  
 ED Entered STN: 16 Nov 1984

CN 5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)

OTHER NAMES:

CN ( $\pm$ )-Citalopram hydrobromide

CN Apertia

CN Celexa

CN Cipram

CN Cipramil

CN Citalopram hydrobromide

CN Elopram

CN Lu 10-171B

CN Lupram

CN Prisadal

CN Sepram

CN Seropram

MF C20 H21 F N2 O . Br H

CI COM

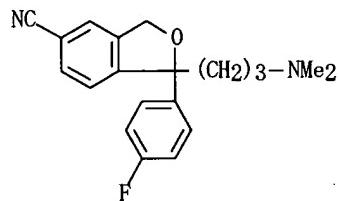
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, DIOGENES, HSDB\*, IFICDB, IFIPAT, IFIUDB, IMSPATENTS, IMSRESEARCH, IPA, MRCK\*, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

CRN (59729-33-8)



● HBr

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

81 REFERENCES IN FILE CA (1907 TO DATE)

81 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 110 tot

L10 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN

RN 488148-14-7 REGISTRY

ED Entered STN: 10 Feb 2003

CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, (1S)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (S)-(+)-1-(4-Fluorophenyl)-1-[3-(dimethylamino)propyl]-5-bromophthalane

FS STEREOSEARCH

MF C19 H21 Br F N O

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (+).

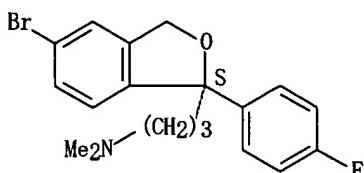
- IT 59729-32-7P, Citalopram hydrobromide 59729-33-8P  
, 1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-  
isobenzofurancarbonitrile  
RL: IMF (Industrial manufacture); SPN (Synthetic  
preparation); PREP (Preparation)  
(process for the preparation of citalopram via cyanation of the  
corresponding chloride or bromide precursor)
- IT 60-29-7, Diethyl ether, uses 67-63-0, Isopropanol, uses 67-64-1,  
Acetone, uses 71-23-8, n-Propanol, uses 108-88-3, Toluene, uses  
110-82-7, Cyclohexane, uses 110-86-1, Pyridine, uses 141-78-6, Ethyl  
acetate, uses 142-82-5, n-Heptane, uses 1330-20-7, Xylene, uses  
27175-64-0, Lutidine  
RL: NUU (Other use, unclassified); USES (Uses)  
(process for the preparation of citalopram via cyanation of the  
corresponding chloride or bromide precursor)
- IT 109-54-6, Dimethylaminopropyl chloride 143-33-9, Sodium cyanide  
151-50-8, Potassium cyanide 352-13-6, 4-Fluorophenyl magnesium bromide  
460-00-4, 4-Fluorobromobenzene 544-92-3, Cuprous cyanide 19070-16-7  
64169-34-2, 5-Bromophthalide 64169-39-7 561304-25-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(process for the preparation of citalopram via cyanation of the  
corresponding chloride or bromide precursor)
- IT 1314-56-3, Phosphorus pentoxide, reactions 7681-11-0, Potassium iodide,  
reactions 10025-87-3, Phosphorus oxychloride  
RL: RGT (Reagent); RACT (Reactant or reagent)  
(process for the preparation of citalopram via cyanation of the  
corresponding chloride or bromide precursor)

=> d all hitrn 169 tot

L69 ANSWER 1 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:691476 HCPLUS  
DN 141:207048  
ED Entered STN: 25 Aug 2004  
TI Preparation of pure citalopram  
IN Kaushik, Vipin Kumar; Rao, Divvela Venkata Naga Srinivasa; Handa, Vijay  
Kumar; Sivakumaran, Meenakshisunderam  
PA Aurobindo Pharma Ltd., India  
SO U.S., 3 pp.  
CODEN: USXXAM  
DT Patent  
LA English  
IC ICM C07D307-78  
NCL 549467000; 549469000  
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

FAN. CNT 1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6781003	B1	20040824	US 2003-456135		20030609
PRAI US 2003-456135			20030609		

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6781003	ICM	C07D307-78		
	NCL	549467000; 549469000		
US 6781003	ECLA	C07D307/81		
OS CASREACT	141:207048			
GI				

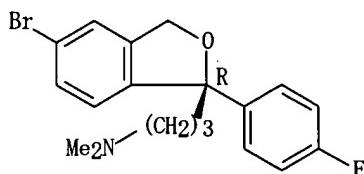


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 488148-13-6 REGISTRY  
 ED Entered STN: 10 Feb 2003  
 CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, (1R)- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN (R)-(-)-1-(4-Fluorophenyl)-1-[3-(dimethylamino)propyl]-5-bromophthalane  
 FS STEREOSEARCH  
 MF C19 H21 Br F N O  
 SR CA  
 LC STN Files: CA, CAPLUS

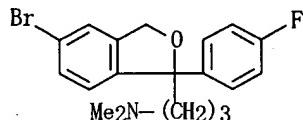
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 479065-02-6 REGISTRY  
 ED Entered STN: 15 Jan 2003  
 CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, hydrobromide (9CI) (CA INDEX NAME)  
 MF C19 H21 Br F N O . Br H  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT  
 CRN (64169-39-7)



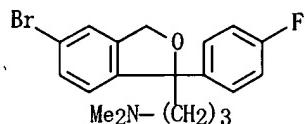
● HBr

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64372-43-6 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 MF C19 H21 Br F N O . C2 H2 O4  
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

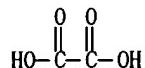
CM 1

CRN 64169-39-7  
 CMF C19 H21 Br F N O



CM 2

CRN 144-62-7  
 CMF C2 H2 O4



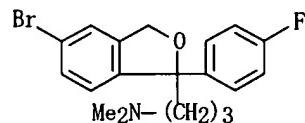
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-40-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)  
 MF C19 H21 Br F N O . x C2 H2 O4  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

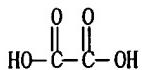
CM 1

CRN 64169-39-7  
 CMF C19 H21 Br F N O



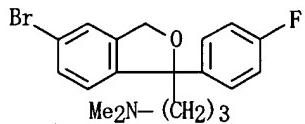
CM 2

CRN 144-62-7  
 CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-39-7 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 1-Isobenzofuranpropanamine, 5-bromo-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 1-(4-Fluorophenyl)-1-(3-dimethylaminopropyl)-5-bromophthalane  
 CN 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran  
 FS 3D CONCORD  
 DR 561304-26-5  
 MF C19 H21 Br F N O  
 CI COM  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)

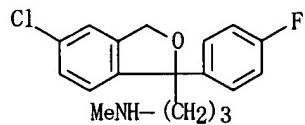


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

20 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 20 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 111 tot

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 561304-25-4 REGISTRY  
 ED Entered STN: 06 Aug 2003  
 CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N-methyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H19 Cl F N O  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

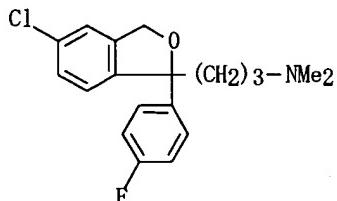


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 113 tot

L13 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-47-7 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)  
 MF C19 H21 Cl F N O . Cl H  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL  
 CRN (64169-45-5)



● HCl

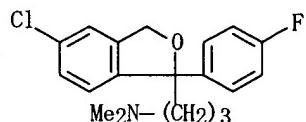
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L13 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-46-6 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)  
 MF C19 H21 Cl F N O . x C2 H2 O4  
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

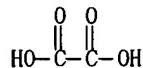
CM 1

CRN 64169-45-5  
 CMF C19 H21 Cl F N O



CM 2

CRN 144-62-7  
 CMF C2 H2 O4



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L13 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64169-45-5 REGISTRY  
 ED Entered STN: 16 Nov 1984

CN 1-Isobenzofuranpropanamine, 5-chloro-1-(4-fluorophenyl)-1,3-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)

## OTHER NAMES:

CN 1-(4-Fluorophenyl)-1-(3-dimethylaminopropyl)-5-chlorophthalane

CN Lu 10-134C

FS 3D CONCORD

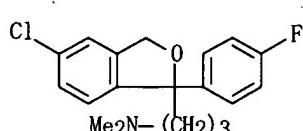
DR 843660-63-9

MF C19 H21 Cl F N O

CI COM

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

12 REFERENCES IN FILE CA (1907 TO DATE)

12 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 117 tot

L17 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN

RN 526204-73-9 REGISTRY

ED Entered STN: 06 Jun 2003

CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (9CI)  
(CA INDEX NAME)

FS STEREOSEARCH

MF C19 H19 F N2 O . C4 H6 O6

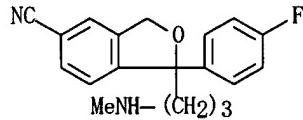
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

CRN 62498-67-3

CMF C19 H19 F N2 O

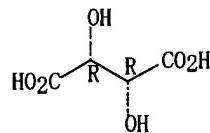


CM 2

CRN 87-69-4

CMF C4 H6 O6

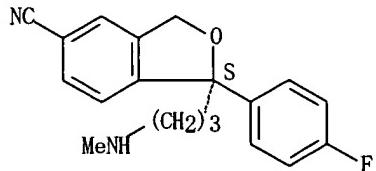
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 144025-14-9 REGISTRY  
 ED Entered STN: 21 Oct 1992  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (1S)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (S)-  
 OTHER NAMES:  
 CN (S)-(+)-N-Demethylcitalopram  
 CN (S)-1-(3-Methylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile  
 CN (S)-Desmethylcitalopram  
 FS STEREOSEARCH  
 MF C19 H19 F N2 O  
 SR CA  
 LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, TOXCENTER,  
 USPATFULL  
 (\*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

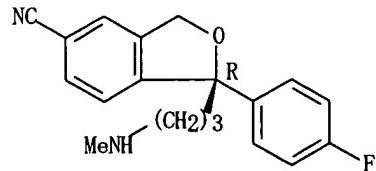


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

25 REFERENCES IN FILE CA (1907 TO DATE)  
 25 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 144010-85-5 REGISTRY  
 ED Entered STN: 16 Oct 1992  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (1R)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, (R)-  
 OTHER NAMES:  
 CN (R)-(-)-N-Demethylcitalopram  
 CN (R)-Desmethylcitalopram  
 FS STEREOSEARCH  
 MF C19 H19 F N2 O  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)

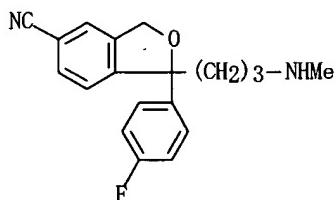
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

19 REFERENCES IN FILE CA (1907 TO DATE)  
 19 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 97743-99-2 REGISTRY  
 ED Entered STN: 24 Aug 1985  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Lu 11-109C  
 MF C19 H19 F N2 O . Cl H  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (62498-67-3)



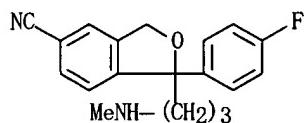
● HCl

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 62498-68-4 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 MF C19 H19 F N2 O . C2 H2 O4  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)

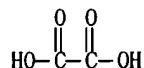
CM 1

CRN 62498-67-3  
 CMF C19 H19 F N2 O



CM 2

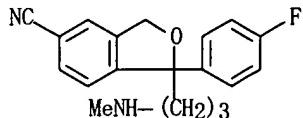
CRN 144-62-7  
 CMF C2 H2 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 62498-67-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarbonitrile, 1-(4-fluorophenyl)-1,3-dihydro-1-[3-(methylamino)propyl]- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN ( $\pm$ )-N-Demethylcitalopram  
 CN Demethylcitalopram  
 CN Desmethylcitalopram  
 CN Lu 11-109  
 CN Norcitalopram  
 CN Rac-Desmethylcitalopram  
 FS 3D CONCORD  
 DR 144070-76-8  
 MF C19 H19 F N2 O  
 CI COM  
 LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CAPLUS,  
 CASREACT, CHEMLIST, DDFU, DRUGU, EMBASE, IPA, MEDLINE, TOXCENTER,  
 USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

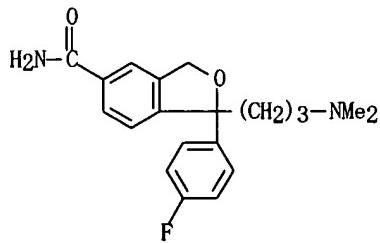


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

108 REFERENCES IN FILE CA (1907 TO DATE)  
 110 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 119 tot

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 64372-56-1 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 5-Isobenzofurancarboxamide, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H23 F N2 O2  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)  
 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 145 tot

L45 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 7681-11-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Antistrumin  
 CN Asmofug E  
 CN Ceoiodin  
 CN Iodostin  
 CN Jodid  
 CN K1-N  
 CN Kaiod  
 CN Knollide  
 CN NSC 77362  
 CN Pherajod  
 CN **Potassium iodide**  
 CN Potassium monoiodide  
 CN Thryo-Block  
 CN Thyrojod  
 DR 59216-96-5, 106449-25-6, 61456-02-8, 39448-53-8  
 MF I K  
 CI COM  
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BIOPHARMA, BIOSIS,  
 BIOTECHNO, CA, CABAB, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CIN, CSHEM, CSNB, DDFU, DETHERM\*, DIOGENES,  
 DIPPR\*, DRUGU, EMBASE, GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA,  
 MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC, PDLCOM\*, PIRA, PROMT, RTECS\*,  
 TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

I-K

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

19901 REFERENCES IN FILE CA (1907 TO DATE)  
 199 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 19915 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d ide 148 tot

L48 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 438043-97-1 REGISTRY  
 ED Entered STN: 10 Jul 2002  
 CN Copper cyanide (63Cu(C15N)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS

63Cu-C≡15N

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 438043-96-0 REGISTRY  
 ED Entered STN: 10 Jul 2002

CN Copper cyanide (63Cu(13CN)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS

63Cu-13C≡N

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 438043-95-9 REGISTRY  
 ED Entered STN: 10 Jul 2002  
 CN Copper cyanide (63Cu(CN)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS

65Cu-C≡N

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 438043-94-8 REGISTRY  
 ED Entered STN: 10 Jul 2002  
 CN Copper cyanide (63Cu(CN)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS

63Cu-C≡N

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 204571-13-1 REGISTRY  
 ED Entered STN: 24 Apr 1998  
 CN Copper cyanide (Cu(C15N)) (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Cuprous cyanide-15N  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS, CHEMCATS

Cu-C≡15N

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 199450-10-7 REGISTRY  
 ED Entered STN: 07 Jan 1998  
 CN Copper cyanide (Cu(13C15N)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHM

Cu-13C≡15N

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 188592-60-1 REGISTRY  
 ED Entered STN: 24 Apr 1997  
 CN Copper cyanide (Cu(NC)), monohydrogen (9CI) (CA INDEX NAME)  
 MF C Cu N . H  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER  
 CRN (147023-48-1)

<sup>+</sup>Cu—N≡C—

● H<sup>+</sup>

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 147023-48-1 REGISTRY  
 ED Entered STN: 16 Apr 1993  
 CN Copper cyanide (Cu(NC)) (9CI) (CA INDEX NAME)  
 MF C Cu N  
 CI CCS, COM  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

<sup>+</sup>Cu—N≡C—

3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 93596-81-7 REGISTRY  
 ED Entered STN: 18 Dec 1984  
 CN Copper cyanide (Cu(13CN)) (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Cuprous cyanide-13C  
 MF C Cu N  
 LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM

Cu—<sup>13</sup>C≡N

11 REFERENCES IN FILE CA (1907 TO DATE)  
 11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 17410-52-5 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Copper cyanide (Cu(14CN)) (8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Copper(I) [14C]cyanide  
 CN Cuprous cyanide-14C  
 CN Cuprous cyanide-14C (Cu14CN)  
 CN Hydrocyanic-14C acid, copper(1+) salt  
 DR 98259-65-5, 35947-46-7, 68378-43-8, 78825-27-1  
 MF C Cu N  
 LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPATFULL

Cu- $^{14}\text{C}\equiv\text{N}$ 

29 REFERENCES IN FILE CA (1907 TO DATE)  
 29 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L48 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 6023-28-5 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Copper cyanide ( $\text{Cu}(\text{CN})$ ), monoammoniate (8CI) (CA INDEX NAME)  
 MF C Cu N . H3 N  
 LC STN Files: GMELIN\*  
     (\*File contains numerically searchable property data)  
 CRN (544-92-3)

Cu- $\text{C}\equiv\text{N}$ ● NH<sub>3</sub>

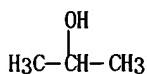
L48 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 544-92-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Copper cyanide ( $\text{Cu}(\text{CN})$ ) (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Copper cyanide  
 CN Copper monocyanide  
 CN Copper(1+) cyanide  
 CN Copper(I) cyanide  
 CN Cupricin  
 CN Cuprous cyanide  
 DR 13092-67-6  
 MF C Cu N  
 CI COM  
 LC STN Files: ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,  
     CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM, CSNB,  
     DETERHM\*, GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, MRCK\*, MSDS-OHS,  
     NIOSHTIC, PDLCOM\*, PROMT, PS, RTECS\*, SYNTHLINE, TOXCENTER, USPAT2,  
     USPATFULL  
     (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

Cu- $\text{C}\equiv\text{N}$ 

1445 REFERENCES IN FILE CA (1907 TO DATE)  
 16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1447 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 39 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=&gt; =&gt; d ide 163 tot

L63 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 70504-57-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, aluminum nickel(2+) salt (8:2:1) (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Nickel bis(tetraisopropanolatealuminate(1-))  
 MF C3 H8 O . 1/4 Al . 1/8 Ni  
 LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL  
 CRN (67-63-0)

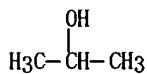


●1/4 Al

●1/8 Ni(II)

8 REFERENCES IN FILE CA (1907 TO DATE)  
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

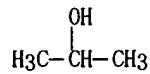
L63 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 30429-72-2 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 2-Propanol, holmium(3+) salt (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Isopropanol, holmium(3+) salt  
MF C3 H8 O . 1/3 Ho  
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL  
CRN (67-63-0)



●1/3 Ho(III)

9 REFERENCES IN FILE CA (1907 TO DATE)  
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

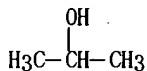
L63 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 6831-82-9 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 2-Propanol, potassium salt (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Isopropyl alcohol, potassium salt (8CI)  
CN Potassium isopropoxide (6CI, 7CI)  
OTHER NAMES:  
CN Potassium isopropanolate  
CN Potassium isopropylate  
MF C3 H8 O . K  
CI COM  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM\*, GMELIN\*, IFICDB, IFIPAT,  
IFIUDB, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
Other Sources: EINECS\*\*  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)  
CRN (67-63-0)



● K

170 REFERENCES IN FILE CA (1907 TO DATE)  
 171 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 14 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

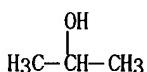
L63 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 6742-69-4 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, ytterbium(3+) salt (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol, ytterbium(3+) salt (8CI)  
 CN Ytterbium isopropoxide (Yb(OC<sub>3</sub>H<sub>7</sub>)<sub>3</sub>) (7CI)  
 OTHER NAMES:  
 CN **Tris(isopropanolato)ytterbium**  
 CN **Tris(isopropoxo)ytterbium**  
 CN **Ytterbium triisopropoxide**  
 MF **C<sub>3</sub> H<sub>8</sub> O . 1/3 Yb**  
 CI COM  
 LC STN Files: CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM,  
 GMELIN\*, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 CRN (67-63-0)



●1/3 Yb(III)

79 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 80 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

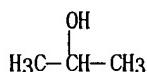
L63 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 2388-10-5 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, lithium salt (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol, lithium salt (8CI)  
 CN Lithium isopropoxide (6CI, 7CI)  
 OTHER NAMES:  
 CN **Isopropanol lithium salt**  
 CN **Isopropoxylithium**  
 CN **Lithium isopropanolate**  
 CN **Lithium isopropylate**  
 MF **C<sub>3</sub> H<sub>8</sub> O . Li**  
 LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN\*, IFICDB, IFIPAT, IFIUDB,  
 TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 CRN (67-63-0)



● Li

168 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 168 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 683-60-3 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, sodium salt (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol, sodium salt (8CI)  
 CN Sodium isopropoxide (6CI, 7CI)  
 OTHER NAMES:  
 CN Isopropanol sodium salt  
 CN Isopropoxysodium  
 CN Sodium isopropanolate  
 CN Sodium isopropyl oxide  
 CN Sodium isopropylate  
 MF C<sub>3</sub> H<sub>8</sub> O . Na  
 CI COM  
 LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM\*, GMELIN\*, IFICDB, IFIPAT,  
 IFIUDB, TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 CRN (67-63-0)

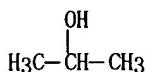


● Na

543 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 545 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 32 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 555-31-7 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, aluminum salt (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol, aluminum salt (8CI)  
 OTHER NAMES:  
 CN AIPD  
 CN Aliso  
 CN Aluminium isopropoxide  
 CN Aluminum 2-propoxide  
 CN Aluminium isopropanolate  
 CN Aluminum isopropionate  
 CN Aluminum isopropoxide  
 CN Aluminum isopropoxide (1:3)  
 CN Aluminum isopropylate  
 CN Aluminum isopropylate (Al(OC<sub>3</sub>H<sub>7</sub>)<sub>3</sub>)  
 CN Aluminum sec-propanolate  
 CN Aluminum triisopropoxide  
 CN Aluminum triisopropylate  
 CN Aluminum tris(iso-propoxide)  
 CN Aluminum tris(isopropoxide)  
 CN Aluminum tris(isopropylate)  
 CN Aluminum tris(sec-propoxide)  
 CN Aluminum(3+) isopropoxide  
 CN Isopropanol aluminum salt  
 CN Manalox 130  
 CN PADM  
 CN Triisopropoxyaluminum

CN Triisopropyl aluminate  
 CN Triisopropoxyaluminum  
 CN Tris(isopropoxy)aluminum  
 DR 12343-27-0, 95797-38-9, 51796-09-9, 78423-41-3, 188398-62-1, 245654-30-2,  
 301192-92-7, 358732-16-8, 365494-41-3  
 MF C<sub>3</sub> H<sub>8</sub> O . 1/3 A1  
 CI COM  
 LC STN Files: AGRICOLA, BEILSTEIN\*, BIOPHARMA, BIOSIS, CA, CAOLD, CAPLUS,  
 CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSHEM, DETHERM\*,  
 ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN\*, HSDB\*, IFICDB,  
 IFIPAT, IFIUDB, IPA, MRCK\*, MSDS-OHS, PROMT, PS, RTECS\*, SPECINFO,  
 TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 CRN (67-63-0)



●1/3 A1

3870 REFERENCES IN FILE CA (1907 TO DATE)  
 207 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 3873 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 78 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 546-68-9 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol, titanium(4+) salt (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol, titanium(4+) salt (8CI)  
 CN Titanium isopropoxide (Ti(OC<sub>3</sub>H<sub>7</sub>)<sub>4</sub>) (7CI)  
 OTHER NAMES:  
 CN 5N  
 CN 5N (titanate)  
 CN A 1  
 CN A 1 (titanate)  
 CN Isopropyl orthotitanate  
 CN Isopropyl titanate(IV) ((C<sub>3</sub>H<sub>7</sub>O)<sub>4</sub>Ti)  
 CN Orgatix TA 10  
 CN TA 10  
 CN Tetraisopropanolatotitanium  
 CN Tetraisopropoxytitanium  
 CN Tetraisopropoxytitanium(IV)  
 CN Tetraisopropyl orthotitanate  
 CN Tetraisopropyl titanate  
 CN Tetrakis(isopropanato)titanium  
 CN Tetrakis(isopropoxy)titanium  
 CN Tetrakis(isopropylato)titanium(IV)  
 CN Tetrakis(isopropoxy)titanium  
 CN Tilcom TIPT  
 CN Titanium isopropoxide  
 CN Titanium isopropylate  
 CN Titanium tetraisopropoxide  
 CN Titanium tetraisopropylate  
 CN Titanium tetrakis(isopropoxide)  
 CN Titanium tetrakis(isopropoxide)  
 CN Titanium(4+) isopropoxide  
 CN Titanium(IV) isopropoxide  
 CN Titanium, tetrakis(1-methylethoxy)-  
 CN TPT  
 CN Tyzor TPT  
 CN Vertec TIPT

DR 505093-57-2, 176680-01-6, 167709-32-2, 128796-34-9, 131530-94-4,  
 94340-28-0, 3651-85-2, 119651-13-7, 112797-74-7, 73264-97-8, 71515-81-6,  
 147809-57-2, 50336-56-6, 118815-04-6, 186518-71-8, 187601-75-8,  
 195382-13-9, 198699-88-6, 210407-18-4, 216859-04-0, 244173-55-5,  
 245654-31-3, 255839-65-7, 259264-35-2, 310882-94-1, 347859-73-8,  
 366477-01-2, 408306-55-8, 518050-49-2

MF C3 H8 O . 1/4 Ti

CI COM

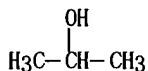
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA,  
 CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST,  
 CIN, CSCHEM, CSNB, DETHERM\*, GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB,  
 MEDLINE, MRCK\*, MSDS-OHS, PIRA, PROMT, RTECS\*, TOXCENTER, USPAT2,  
 USPATFULL

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

CRN (67-63-0)



●1/4 Ti(IV)

8443 REFERENCES IN FILE CA (1907 TO DATE)  
 454 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 8458 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

RN 71-23-8 REGISTRY

ED Entered STN: 16 Nov 1984

CN 1-Propanol (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Propyl alcohol (8CI)

OTHER NAMES:

CN 1-Hydroxypropane

CN Ethylcarbinol

CN n-Propanol

CN n-Propyl alcohol

CN NSC 30300

CN Optal

CN Osmosol extra

CN Propanol

FS 3D CONCORD

MF C3 H8 O

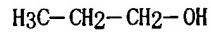
CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
 BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN,  
 CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU,  
 DETHERM\*, DIPPR\*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT,  
 ENCOMPPAT2, GMELIN\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA,  
 MEDLINE, MRCK\*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM\*, PIRA, PROMT, PS,  
 RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2,  
 USPATFULL, VETU, VTB

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

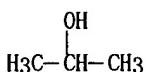
(\*\*Enter CHEMLIST File for up-to-date regulatory information)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

30692 REFERENCES IN FILE CA (1907 TO DATE)  
 465 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 30718 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L63 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 67-63-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN 2-Propanol (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Isopropyl alcohol (8CI)  
 OTHER NAMES:  
 CN 1-Methylethanol  
 CN 1-Methylethyl alcohol  
 CN 2-Hydroxypropane  
 CN 2-Propyl alcohol  
 CN Alcojel  
 CN Alcosolve 2  
 CN Autosept  
 CN Avantin  
 CN Avantine  
 CN Combi-Schutz  
 CN Dimethylcarbinol  
 CN Hartosol  
 CN Imsol A  
 CN IPA  
 CN IPS 1  
 CN IPS 1 (alcohol)  
 CN iso-Propanol  
 CN iso-Propyl alcohol  
 CN Isohol  
 CN Isopropanol  
 CN Lutosol  
 CN n-Propan-2-ol  
 CN NSC 135801  
 CN Petrohol  
 CN PRO  
 CN Propol  
 CN sec-Propanol  
 CN sec-Propyl alcohol  
 CN Sterisol Hand Disinfectant  
 CN Takineocol  
 CN Tokuso IPA  
 CN Virahol  
 FS 3D CONCORD  
 DR 8013-70-5  
 MF C3 H8 O  
 CI COM  
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOBUSINESS,  
 BIOSIS, BIOTECHNO, CA, CABAB, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB,  
 CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB,  
 DDFU, DETHERM\*, DIOGENES, DIPPR\*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2,  
 ENCOMPPAT, ENCOMPPAT2, GMELIN\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB,  
 IPA, MEDLINE, MRCK\*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM\*, PIRA,  
 PROMT, PS, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USAN,  
 USPAT2, USPATFULL, VETU, VTB  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

48960 REFERENCES IN FILE CA (1907 TO DATE)  
 816 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 49038 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his full

(FILE 'HOME' ENTERED AT 13:27:33 ON 11 APR 2005)

FILE 'HCAPLUS' ENTERED AT 13:27:40 ON 11 APR 2005

L1 1 SEA ABB=ON PLU=ON US20050043550/PN  
 L2 1 SEA ABB=ON PLU=ON (IN2002-MU847 OR IN2002-MU18 OR IN2002-MU10  
     OR W2003-ING)/AP, PRN  
 L3 1 SEA ABB=ON PLU=ON (L1 OR L2)

FILE 'REGISTRY' ENTERED AT 13:29:08 ON 11 APR 2005

L4 FILE 'HCAPLUS' ENTERED AT 13:29:10 ON 11 APR 2005  
 TRA L3 1- RN : 28 TERMS

FILE 'REGISTRY' ENTERED AT 13:29:10 ON 11 APR 2005

L5 28 SEA ABB=ON PLU=ON L4  
 L6 QUE ABB=ON PLU=ON (PMS OR MAN OR IDS)/CI OR UNSPECIFIED OR  
     COMPOUND OR COMPD OR (D OR T)/ELS  
 L7 27 SEA ABB=ON PLU=ON C20H21FN20 AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
 L8 22 SEA ABB=ON PLU=ON L7 NOT L6  
     SEL RN 1-4 7-22 L8  
 L9 20 SEA ABB=ON PLU=ON (107190-73-8/BI OR 128196-01-0/BI OR  
     128196-02-1/BI OR 129356-76-9/BI OR 134915-04-1/BI OR 135021-05  
     -5/BI OR 141258-68-6/BI OR 207559-01-1/BI OR 219861-08-2/BI OR  
     219861-53-7/BI OR 481047-49-8/BI OR 481047-50-1/BI OR 490037-56  
     -4/BI OR 500733-84-6/BI OR 59729-32-7/BI OR 59729-33-8/BI OR  
     64169-59-1/BI OR 64372-50-5/BI OR 64372-51-6/BI OR 85118-27-0/B  
     I) AND L8  
     D SCA  
 L10 6 SEA ABB=ON PLU=ON C19H21BRFNO AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
     D SCA  
 L11 1 SEA ABB=ON PLU=ON C18H19CLFNO AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
     D SCA  
 L12 6 SEA ABB=ON PLU=ON C19H21CLFNO AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
     D STR TOT  
     SEL RN 4-6 L12  
 L13 3 SEA ABB=ON PLU=ON (64169-45-5/BI OR 64169-46-6/BI OR  
     64169-47-7/BI) AND L12  
 L14 8 SEA ABB=ON PLU=ON C19H19FN20 AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
     D SCA  
 L15 7 SEA ABB=ON PLU=ON L14 NOT (D OR T)/ELS  
 L16 7 SEA ABB=ON PLU=ON L15 AND METHYLAMINO  
 L17 6 SEA ABB=ON PLU=ON L16 NOT DIMETHYLAMINO  
 L18 7 SEA ABB=ON PLU=ON C20H23FN202 AND OC4-C6/ES AND 46.150.18/RID  
     AND NR=3  
     D SCA  
 L19 1 SEA ABB=ON PLU=ON ISOBENZOFURANCARBOXAMIDE AND L18

FILE 'HCAPLUS' ENTERED AT 13:53:58 ON 11 APR 2005

L20 93 SEA ABB=ON PLU=ON (L9 OR ?CITALOPRAM/BI OR CIPRALEX OR  
     LEXAPRO OR LU (1A) (260540 OR 26 (1A) 0540 OR 26 (1A) 054?) OR  
     LU26054? OR LU26 (1A) 540 OR BONITRILE OR LU10171 OR LU10 (1A)  
     171 OR LU (1A) (10171 OR 10 (1A) 171) OR NITRALAPRAM OR  
     APERTIA OR CELEXA OR CIPRAM) (L) PREP+NT/RL  
 L21 0 SEA ABB=ON PLU=ON (CIPRAMIL# OR ELOPRAM# OR LUPRAM OR  
     PRISDAL# OR SEPRAM# OR SEROPRAM# OR LU10171B OR LU10 (1A) 171B  
     OR LU(1A) (10171B OR 10 (1A) 171B OR 10171 (1A) B OR 10 (1A)

L22 32 SEA ABB=ON PLU=ON L10 OR L11 OR L13 OR FLUOROPHENYL (2A) (DIME THYLAMINO OR DIMETHYL (1A) AMINO OR DI (1A) METHYL (1A) AMINO OR DI (1A) METHYLAMINO) (1A) PROPYL (1A) BROMOPHTHALENE

L23 412 SEA ABB=ON PLU=ON BROMO (1A) (DIMETHYLAMINO OR DIMETHYL (1A) AMINO OR DI (1A) (METHYLAMINO OR METHYL (1A) AMINO) (2A) FLUOROPHENYL (2A) (DIHYDROISOBENZOFURAN OR DI (1A) (HYDROISOBENZ OFURAN OR HYDRO (1A) (ISOBENZOFURAN OR ISO (1A) (BENZOFURAN OR BENZO(1A)FURAN))))

L24 3 SEA ABB=ON PLU=ON LU10134C OR LU (1A) (10134C OR 10 (1A) 134C OR 10 (1A) 134 (1A) C)

L25 26 SEA ABB=ON PLU=ON L20 AND (L22 OR L23 OR L24)

L26 QUE ABB=ON PLU=ON PY<=2003 OR AY<=2003 OR PRY<=2003

E RAJAMANNAR T/AU

L27 20 SEA ABB=ON PLU=ON ("RAJAMANNAR T"/AU OR "RAJAMANNAR THENNATI" /AU)  
E SRINVASU K/AU  
E SRINIVASU K/AU

L28 6 SEA ABB=ON PLU=ON "SRINIVASU K"/AU  
E PATEL N/AU

L29 411 SEA ABB=ON PLU=ON ("PATEL N"/AU OR "PATEL N K"/AU OR "PATEL N S"/AU)  
E PATEL NILESH/AU

L30 6 SEA ABB=ON PLU=ON ("PATEL NILESHKUMAR"/AU OR "PATEL NILESHKUM AR SURESHBAI"/AU OR "PATEL NILESHKUMAR SURESHBAI"/AU OR "PATEL NILI"/AU)  
E REJENDRAN C/AU  
D BIB L3  
E CHINAPILLAI R/AU  
E CHINNAPILLAI R/AU

L31 1 SEA ABB=ON PLU=ON "CHINNAPILLAI RAJENDRAN"/AU

L32 63 SEA ABB=ON PLU=ON (SUN AND PHARM? AND IND?)/CS, PA

L33 2 SEA ABB=ON PLU=ON L25 AND (L27 OR L28 OR L29 OR L30 OR L31 OR L32)

L34 24 SEA ABB=ON PLU=ON L25 NOT L32

L35 133 SEA ABB=ON PLU=ON L17 OR L19 OR (ISOBENZOFURANCARBONITRILE OR ISO (1A) (BENZOFURANCARBONITRILE OR BENZO (1A) (FURANCARBONIT RILE OR FURAN (1A) CARBONITRILE)) OR (ISOBENZOFURAN OR ISOBENZO (1A) FURAN) (1A) (CARBONITRILE OR CARBO (1A) NITRILE)) (2A) FLUOROPHENYL (2A) DIHYDRO

L36 3 SEA ABB=ON PLU=ON L35 (2A) (METHYLAMINOPROPYL OR (METHYLAMINO OR METHYL (1A) AMINO) (1A)PROPYL) OR DEMETHYLCTALPRAM# OR DEMETHYLCTALOPRAM# OR NORCITALPRAM# OR LU11109 OR LU (1A) (11109 OR 11 (1A) 109)  
D SCA

L37 3 SEA ABB=ON PLU=ON L34 AND (L35 OR L36)

L38 21 SEA ABB=ON PLU=ON (L9 OR ?CITALOPRAM/BI OR CIPRALEX OR LEXAPRO OR LU (1A) (260540 OR 26 (1A) 0540 OR 26(1A) 054?) OR LU26054? OR LU26 (1A) 540 OR BONITRILE OR LU10171 OR LU10 (1A) 171 OR LU (1A) (10171 OR 10 (1A) 171) OR NITRALAPRAM OR APERTIA OR CELEXA OR CIPRAM) (L) PUR/RL

L39 1 SEA ABB=ON PLU=ON L38 AND (L27 OR L28 OR L29 OR L30 OR L31 OR L32)

L40 20 SEA ABB=ON PLU=ON L38 NOT L39  
E CRYSTALLIZ/CT  
E E5+ALL

L41 117878 SEA ABB=ON PLU=ON CRYSTALLIZATION+NT/CT  
E E30  
E E3+ALL

L42 89849 SEA ABB=ON PLU=ON CRYSTALS+NT/CT  
E PRECIPITATION (CHEMICAL)/CT  
E E3+ALL

L43 25533 SEA ABB=ON PLU=ON "PRECIPITATION (CHEMICAL)"+OLD, NT/CT

L44 3 SEA ABB=ON PLU=ON L40 AND (L41 OR L42 OR L43)

FILE 'REGISTRY' ENTERED AT 15:19:08 ON 11 APR 2005.

E POTASSIUM IODIDE/CN

L45 1 SEA ABB=ON PLU=ON "POTASSIUM IODIDE"/CN

E CUPROUS CYANIDE/CN

L46 1 SEA ABB=ON PLU=ON "CUPROUS CYANIDE"/CN

D SCA  
L47 18 SEA ABB=ON PLU=ON CCUN AND COPPER (1A) CYANIDE  
L48 12 SEA ABB=ON PLU=ON L47 NOT L6

FILE 'HCAPLUS' ENTERED AT 15:24:06 ON 11 APR 2005  
L49 91001 SEA ABB=ON PLU=ON L46 OR ?POTASSIUM/BI (1A) ?IODIDE/BI OR  
ANTISTRUMIN# OR ASMOFUG# OR CEOIODIN# OR IODOSTIN# OR JODID OR  
KI OR K1N OR K1 (1A) N OR KAID# OR KNOLLIDE OR NSC77632 OR  
NSC (1A) (77632 OR 77(1A)632) OR PHERAJOD# OR THRYOBLOCK OR  
THYRO (1A) BLOCK OR THYROJOD#  
L50 4727 SEA ABB=ON PLU=ON L48 OR (COPPER OR CUPROUS OR CUPRATE) (2A)  
?CYANIDE/BI OR CUPRICIN#  
L51 24 SEA ABB=ON PLU=ON L25 NOT L33  
L52 3 SEA ABB=ON PLU=ON L51 AND (L35 OR L36)  
L53 3 SEA ABB=ON PLU=ON L37 OR L52  
L54 11 SEA ABB=ON PLU=ON L51 AND L49  
L55 11 SEA ABB=ON PLU=ON L54 AND L50  
E ALCOHOLS/CT  
E E3+OLD, NT1  
L56 QUE ABB=ON PLU=ON ALCOHOLS+OLD, NT1/CT OR ALCOHOL#/CW  
E ISOPROPANOL/CT  
E CYCLOHEXANE/CT  
E E3+ALL  
L57 35276 SEA ABB=ON PLU=ON CYCLOHEXANE/CT  
L58 0 SEA ABB=ON PLU=ON L55 AND L56  
L59 1 SEA ABB=ON PLU=ON L55 AND L57  
D SCA  
D COS

FILE 'REGISTRY' ENTERED AT 15:36:14 ON 11 APR 2005

E ISOPROPANOL/CN  
L60 1 SEA ABB=ON PLU=ON ISOPROPANOL/CN  
D SCA  
L61 71 SEA ABB=ON PLU=ON C3H8O AND (ISOPROPANOL OR N-PROPANOL)  
L62 26 SEA ABB=ON PLU=ON L61 NOT L6  
L63 10 SEA ABB=ON PLU=ON L62 NOT (MXS/CI OR MIXT)

FILE 'HCAPLUS' ENTERED AT 15:39:22 ON 11 APR 2005

L64 QUE ABB=ON PLU=ON L63 OR ?PROPYL/BI (1A) ALCOHOL OR ?ISOPROP?  
/BI OR ?PROPANOL/BI OR TIPT OR HYDROXYPROPANE OR ETHYLCARBINOL  
OR NSC30300 OR NSC (1A) (30300 OR 30 (1A) 300) OR ETHYL (1A)  
CARBINOL OR OPTAL# OR OSMOSAL OR PROPANOL OR METYLETH? OR  
ALCOJEL OR ALCOSOLVE  
L65 7371 SEA ABB=ON PLU=ON AUTOSEPT OR AVANTIN# OR COMBI (1A) SCHUTZ  
OR COMBISCHUTZ OR DIMETHYLCARBINOL OR (DIMETHYL OR DI (1A)  
METHYL) (1A) CARBINOL OR HARTOSOL# OR IPA OR IPS OR LUSOL# OR  
PROPAN (1A) OL OR PETROHOL#  
L66 72 SEA ABB=ON PLU=ON NSC135801 OR NSC (1A) (135801 OR 135 (1A)  
801) OR PROPOL# OR STERISOL# OR TAKINEOCOL# OR TOKUSO OR  
VIRAHOL#  
L67 1 SEA ABB=ON PLU=ON L55 AND (L64 OR L65 OR L66)  
L68 2 SEA ABB=ON PLU=ON L59 OR L67  
D SCA  
L69 8 SEA ABB=ON PLU=ON L44 OR L53 OR L68  
L70 2 SEA ABB=ON PLU=ON L33 OR L39

=> b hcap

FILE 'HCAPLUS' ENTERED AT 15:49:06 ON 11 APR 2005

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FILE COVERS 1907 - 11 Apr 2005 VOL 142 ISS 16  
FILE LAST UPDATED: 10 Apr 2005 (20050410/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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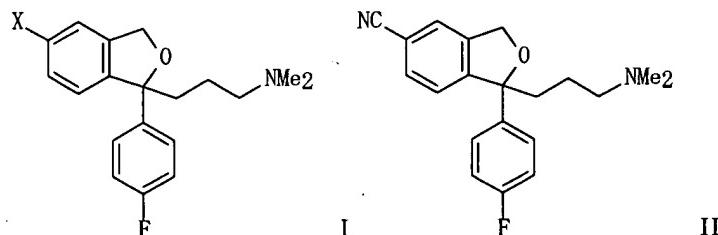
L70 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:1079731 HCAPLUS  
DN 142:56160  
ED Entered STN: 17 Dec 2004  
TI process for purification of citalopram by hydrogenolysis halogenated isobenzofuran impurities  
IN Borase, Ashok Punju; Patel, Nileshkumar Sureshbhai; Kilaru, Srinivasu; Thennati, Rajamannar  
PA Sun Pharmaceuticals Industries Ltd., India  
SO Eur. Pat. Appl., 17 pp.  
CODEN: EPXXDW  
DT Patent  
LA English  
IC ICM C07D307-87  
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 63

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1486492	A2	20041215	EP 2004-291424	20040608
EP 1486492	A3	20050223		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
US 2005004380	A1	20050106	US 2004-865139	20040608
PRAI IN 2003-MU602	A	20030610		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1486492	ICM	C07D307-87
OS MARPAT	142:56160	
GI		



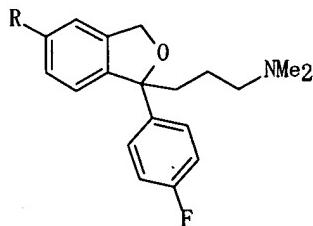
- AB The present invention provides a process for decreasing the content of halogenated isobenzofuran impurities I (X = halo) in citalopram (II) by hydrogenolysis to I (X = H). Thus, 5 g crude citalopram base containing 4.84% of bromo impurity I (X = Br) is dissolved in 50 mL EtOAc, 0.1 g Pd/C and 0.1 g sodium hypophosphite added and the mixture refluxed for 2 h. Anal. showed that the bromo impurity I (X = Br) is absent.
- ST citalopram purifn hydrogenolysis halogenated isobenzofuran impurity
- IT Hydrogenolysis  
(process for purification of citalopram by hydrogenolysis halogenated impurities)
- IT Alcohols, uses

	RL: NUU (Other use, unclassified); USES (Uses) (solvent; process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses RL: CAT (Catalyst use); USES (Uses) (process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	59729-32-7P, Citalopram hydrobromide 59729-33-8P , Citalopram 207559-01-1P, Citalopram oxalate RL: PUR (Purification or recovery); PREP (Preparation) (process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	64169-39-7 RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent) (process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	540-69-2, Ammonium formate 1333-74-0, Hydrogen, reactions 7681-53-0, Sodium hypophosphite RL: RGT (Reagent); RACT (Reactant or reagent) (process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	390817-87-5P RL: SPN (Synthetic preparation); PREP (Preparation) (process for purification of citalopram by hydrogenolysis halogenated impurities)
IT	75-09-2, Dichloromethane, uses 141-78-6, Ethyl acetate, uses 7732-18-5, Water, uses RL: NUU (Other use, unclassified); USES (Uses) (solvent; process for purification of citalopram by hydrogenolysis halogenated impurities)
L70	ANSWER 2 OF 2 HCPLUS COPYRIGHT 2005 ACS on STN
AN	2003:551309 HCPLUS
DN	139:117333
ED	Entered STN: 18 Jul 2003
TI	Process for the preparation of 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile via cyanation of the corresponding chloride or bromide precursors.
IN	Thennati, Rajamannar; Kilaru, Srinivasu; Chinnapillai, Rajendran ; Patel, Nileshkumar Sureshbhai
PA	Sun Pharmaceutical Industries Limited, India
SO	PCT Int. Appl., 41 pp. CODEN: PIXXD2
DT	Patent
LA	English
IC	ICM A61K
CC	27-7 (Heterocyclic Compounds (One Hetero Atom))
FAN. CNT 1	PATENT NO. KIND DATE APPLICATION NO. DATE
PI	WO 2003057132 A2 20030717 WO 2003-IN6 20030107 WO 2003057132 A3 20040226 WO 2003057132 C1 20040415 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI	US 2005043550 A1 20050224 US 2004-500532 20040719 IN 2002-MU10 A 20020107 IN 2002-MU18 A 20020110

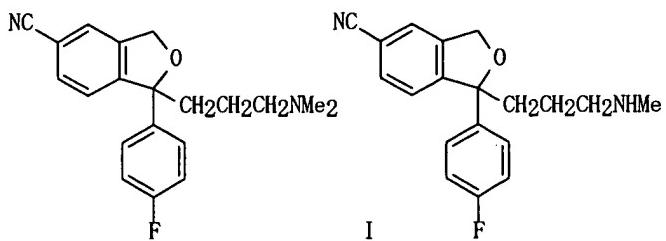
IN 2002-MU847 A 20020930  
WO 2003-IN6 W 20030107

CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2003057132 ICM A61K  
US 2005043550 ECLA C07D307/87B  
OS CASREACT 139:117333; MARPAT 139:117333  
GI



- AB Title compound (I; R = cyano) (citalopram) was prepared by treatment of I (R = Cl, Br) with a cyanide source in the presence of I<sup>-</sup> in an amide, amine, or polyether solvent followed by treatment of the crude product containing 1-[3-(methylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile and 5-carboxamido-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)phthalide impurities with a phosphorus oxyhalide, phosphorus oxide cyanide reversal agent, and purification using a solvent system comprising a hydrocarbon and alc., ester, ether, ketone, or mixture thereof. Thus, citalopram containing 4.7% amide and 0.72% desmethylcitalopram impurities was heated with POCl<sub>3</sub> in PhMe at 70° for 1 h. The mixture was poured into water and pH was adjusted to 2.0-2.5 with aqueous HCl. The PhMe layer was separated and the pH of the aqueous layer was adjusted to 9.0-9.5 with aqueous NH<sub>3</sub> followed by extraction with PhMe to give product containing 0.05% and 0.23% of the amide and desmethylcitalopram resp.
- ST citalopram prepn purifn phosphorus oxychloride;  
halodimethylaminopropylfluorophenyldihydrobenzofuran cyanation
- IT Solvents  
(halogenated; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Cyanation catalysts  
(iodide ion; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Iodides, reactions  
RL: RGT (Reagent); RACT (Reactant or reagent)  
(metal iodides; process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Cyanation  
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT Alcohols, uses  
Amides, uses  
Amines, uses  
Aromatic hydrocarbons, uses  
Esters, uses  
Ethers, uses  
Hydrocarbons, uses  
Ketones, uses  
Nitriles, uses  
Nitro compounds  
Polyethers, uses  
RL: NUU (Other use, unclassified); USES (Uses)  
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)
- IT 62498-67-3P 64372-56-1P  
RL: BYP (Byproduct); PREP (Preparation)  
(process for the preparation of citalopram via cyanation of the corresponding chloride or bromide precursor)



- AB The present invention relates to an industrially advantageous method for the purification of citalopram (I) wherein desmethyl citalopram (II), present in crude citalopram as an impurity, is methylated to produce pure citalopram I. The resulting citalopram product I is isolated as the base or a pharmaceutically acceptable salt thereof. Thus, to crude citalopram (90 g, 0.28 mol) containing desmethyl citalopram (7 %, HPLC), formic acid (98%, 2.7 g) was added followed by aqueous formaldehyde(35%, 2.37 g). The reaction mass was heated at 85-95° for 30 min, cooled to 30°, and diluted with ethanol (900 mL), treated with oxalic acid dihydrate (41.94 g, 0.33 mol), and heated to reflux. The obtained solution was cooled to 20-25° and stirring was continued for 2 h at 20-25°, followed by collecting the product by filtration and recrystn. from ethanol to give highly pure 92 g crystalline citalopram oxalate having HPLC purity 99.7% wherein desmethyl citalopram (impurity) was not detected.
- ST methylation desmethyl citalopram formaldehyde formic acid; citalopram prep
- IT 62498-67-3P, Desmethyl citalopram  
 RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation)  
 ; RACT (Reactant or reagent)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 59729-33-8P, Citalopram  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 59729-32-7P, Citalopram Hydrobromide  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 64-18-6, Formic acid, reactions  
 RL: RGT (Reagent); RACT (Reactant or reagent)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 50-00-0, Formaldehyde, reactions 544-92-3, Cuprous cyanide 6153-56-6, Oxalic acid dihydrate 10035-10-6, Hydrobromic acid, reactions 64169-39-7, 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran 207559-01-1, Citalopram oxalate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant; preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Petersen; US 6258842 B1 2001 HCPLUS  
 (2) Petersen; US 6291689 B1 2001 HCPLUS

IT 62498-67-3P, Desmethyl citalopram  
 RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation)  
 ; RACT (Reactant or reagent)  
 (preparation of pure citalopram by N-methylation of crude

- citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 59729-33-8P, Citalopram  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 59729-32-7P, Citalopram Hydrobromide  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)
- IT 64169-39-7, 5-Bromo-1-(3-dimethylaminopropyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant; preparation of pure citalopram by N-methylation of crude citalopram containing desmethyl citalopram with formaldehyde and formic acid)

L69 ANSWER 2 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2004:546472 HCPLUS  
 DN 141:106278  
 ED Entered STN: 08 Jul 2004  
 TI A process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram  
 IN Petersen, Hans; Dancer, Robert; Christiansen, Brian; Humble, Rikke Eva  
 PA H. Lundbeck A/S, Den.  
 SO PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07C253-34  
 ICS C07D307-87  
 CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 45, 48

FAN.	CNT	1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004056754	A1	20040708	WO 2003-DK907		20031218	
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					

PRAI DK 2002-2004 A 20021223  
 US 2002-436117P P 20021223

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	WO 2004056754	ICM	C07C253-34
		ICS	C07D307-87

AB The invention relates to a process for the preparation of racemic citalopram diol [i.e., citalopram diol means 4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]-3-(hydroxymethyl)benzonitrile] and/or R- or S-citalopram diol, comprising the separation of a non-racemic mixture of R- and S-citalopram diol with more than 50% of one of the enantiomers into a fraction being enriched with S- or R-citalopram diol and a fraction comprising RS-citalopram diol wherein the ratio of R-citalopram diol:S-citalopram diol is equal to 1:1 or closer to 1:1 than in the initial mixture. The method is characterized in that (i) RS-citalopram diol is precipitated from a solution of the initial non-racemic mixture, or R- or S-citalopram diol is

dissolved into a solvent from the initial non-racemic mixture, leaving a residue of RS-citalopram diol, and in that (ii) the residue/precipitate formed is separated from the final solution phase, followed by optional steps of repetition, recrystn., purification, isolation and conversion between free base and salts. The invention also relates to a process for the preparation of RS-citalopram, S-citalopram or R-citalopram (all as free base and/or acid addition salt) comprising the method described above followed by ring closure.

- ST citalopram diol racemic prepn  
 IT **Crystallization**  
 Neutralization  
   **Precipitation (chemical)**  
   **Recrystallization**  
 Resolution (separation)  
   (process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT Alcohols, uses  
 Ketones, uses  
 RL: NUU (Other use, unclassified); USES (Uses)  
   (solvents; process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT 481047-48-7P 488787-59-3P  
 RL: PUR (Purification or recovery); PREP (Preparation)  
   (process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT 64-19-7, Acetic acid, reactions 75-75-2, Methanesulfonic acid 104-15-4, reactions 144-62-7, Oxalic acid, reactions 7647-01-0, Hydrogen chloride, reactions 7664-93-9, Sulfuric acid, reactions 10035-10-6, Hydrogen bromide, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
   (process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT 103146-25-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
   (process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT 717133-25-0P 717133-26-1P 717133-27-2P 717133-28-3P 717133-29-4P  
 717133-30-7P 717133-31-8P 717133-32-9P 717909-60-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
   (process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)  
 IT 60-29-7, Ethyl ether, uses 67-63-0, 2-Propanol, uses 67-64-1, Acetone, uses 75-05-8, Acetonitrile, uses 108-10-1, Methyl isobutyl ketone 108-88-3, Toluene, uses 109-99-9, Thf, uses 141-78-6, Ethyl acetate, uses 7732-18-5, Water, uses  
 RL: NUU (Other use, unclassified); USES (Uses)  
   (solvent; process for the preparation of racemic citalopram diol and/or S- or R-citalopram diols and the use of such diols for the preparation of racemic citalopram R-citalopram and/or S-citalopram)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

- RE  
 (1) H Lundbeck AS; EP 0347066 A1 1989 HCPLUS  
 (2) H Lundbeck AS; WO 03000672 A1 2003 HCPLUS

- L69 ANSWER 3 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2003:777773 HCPLUS  
 DN 139:276808  
 ED Entered STN: 03 Oct 2003  
 TI Transalification process for the preparation of purified citalopram hydrochloride or hydrobromide  
 IN Hamied, Yusuf Khwaja; Kankan, Rajendra N.; Rao, Dharmaraj R.  
 PA Cipla Ltd., India; Wain, Christopher Paul

SO PCT Int. Appl., 10 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D307-87  
 ICS A61K031-343  
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45, 48, 63  
 FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080589	A1	20031002	WO 2003-GB1032	20030311
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1485367	A1	20041215	EP 2003-708344	20030311
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRAI	BR 2003008603	A	20050209	BR 2003-8603	20030311
	GB 2002-6708	A	20020321		
	WO 2003-GB1032	W	20030311		

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	WO 2003080589	ICM	C07D307-87
		ICS	A61K031-343

- AB Purified citalopram hydrochloride or hydrobromide are made by purifying another different citalopram salt (e.g., citalopram besylate by crystallization) and then converting the purified salt to the hydrochloride or hydrobromide.  
 ST transalification prep citalopram hydrochloride; hydrobromide citalopram transalification prep; crystn transalification prep citalopram hydrobromide  
 IT Crystallization  
     (in a transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)  
 IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-64-1, Acetone, uses 78-93-3, MEK, uses 108-10-1, MIBK 108-88-3, Toluene, uses 110-54-3, Hexane, uses 141-78-6, Ethyl acetate, uses 142-82-5, Heptane, uses 7732-18-5, Water, uses  
     RL: NUU (Other use, unclassified); USES (Uses)  
         (crystallization solvent; in a transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)  
 IT 606932-12-1P  
     RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
         (transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)  
 IT 98-11-3, Benzenesulfonic acid, reactions 59729-33-8, Citalopram  
     RL: RCT (Reactant); RACT (Reactant or reagent)  
         (transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)  
 IT 59729-32-7P, Citalopram hydrobromide 85118-27-0P, Citalopram hydrochloride  
     RL: SPN (Synthetic preparation); PREP (Preparation)  
         (transalification process for the preparation of purified citalopram hydrochloride or hydrobromide)

RE. CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

- RE
- (1) Liljegren, K; WO 0180619 A 2001 HCPLUS
  - (2) Paul, W; WO 02070501 A 2002 HCPLUS
  - (3) Petersen, H; WO 0168627 A 2001
  - (4) Sumika Fine Chemicals Co Ltd; EP 1152000 A 2001 HCPLUS

L69 ANSWER 4 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2003:590880 HCPLUS  
 DN 139:133459  
 ED Entered STN: 01 Aug 2003  
 TI Cyanation process for the preparation of citalopram and its extractive purification  
 IN Coppi, Laura; Gasanz Guillen, Yolanda; Campon Pardo, Julio  
 PA Esteve Quimica, S.A., Spain  
 SO U.S. Pat. Appl. Publ., 5 pp.  
 CODEN: USXXCO  
 DT Patent  
 LA English  
 IC C07D307-87  
 NCL 549467000  
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45, 48

## FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003144534	A1	20030731	US 2003-351289	20030124
	US 6635773	B2	20031021		
	ES 2194597	A1	20031116	ES 2002-167	20020125
	ES 2194597	B2	20040801		
	WO 2003062218	A1	20030731	WO 2003-ES37	20030124
		W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		
		RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
	EP 1479673	A1	20041124	EP 2003-706634	20030124
		R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK		
PRAI	ES 2002-167	A	20020125		
	WO 2003-ES37	W	20030124		

## CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	US 2003144534	ICM	C07D307-87
		NCL	549467000
	US 2003144534	ECLA	C07D307/87B
	EP 1479673	ECLA	C07D307/87B
AB	Crude citalopram was prepared the cyanation of 1-[3-(dimethylamine)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-bromoisoindolizofuran with copper cyanide and purified citalopram or one of its salts (e.g., citalopram hydrobromide) was obtained by the extractive purification of citalopram by selective extrns. of citalopram or its salts of its impurities with organic solvents (e.g., toluene and heptane) and water under specific conditions of pH and temperature		
ST	citalopram prepns extractive purifn; hydrobromide citalopram prepns extractive purifn		
IT	Extraction (cyanation process for the preparation of citalopram and its extractive purification)		
IT	Cyanation (cyanation process using copper cyanide and 1-[3-(dimethylamine)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-bromoisoindolizofuran for the preparation of citalopram and its extractive purification)		
IT	Aromatic hydrocarbons, uses RL: NUU (Other use, unclassified); USES (Uses) (extraction solvents; in a cyanation process for the preparation of citalopram and its extractive purification)		
IT	Neutralization (of citalopram base with acids in the preparation of citalopram salts)		

- IT **59729-33-8P, Citalopram**  
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **544-92-3, Copper cyanide 64169-39-7**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **59729-32-7P, Citalopram hydrobromide**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **108-88-3, Toluene, uses 110-54-3, Hexane, uses 110-82-7, Cyclohexane, uses 142-82-5, Heptane, uses 1330-20-7, Xylene, uses 100-88-3**  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (extraction solvent; in a cyanation process for the preparation of citalopram and its extractive purification)
- IT **10035-10-6, Hydrogen bromide, reactions**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (in the preparation of citalopram hydrobromide)
- IT **7732-18-5, Water, uses**  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (solvent; cyanation process for the preparation of citalopram and its extractive purification)
- IT **59729-33-8P, Citalopram**  
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **544-92-3, Copper cyanide 64169-39-7**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **59729-32-7P, Citalopram hydrobromide**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (cyanation process for the preparation of citalopram and its extractive purification)
- IT **110-82-7, Cyclohexane, uses**  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (extraction solvent; in a cyanation process for the preparation of citalopram and its extractive purification)

L69 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2003:32670 HCPLUS  
 DN 138:55856  
 ED Entered STN: 15 Jan 2003  
 TI Process for the preparation of highly pure salts of citalopram  
 IN Satyanarayana, Chava; Venkata, Ramana Rao Chunchu; Jyothi, Basu Abbineni; Hari, Babu Bobepudi  
 PA Matrix Laboratories Limited, India  
 SO Brit. UK Pat. Appl., 18 pp.  
 CODEN: BAXXDU  
 DT Patent  
 LA English  
 IC ICM C07D307-87  
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 63

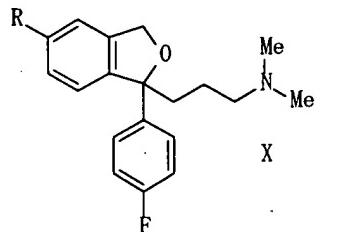
FAN.	CNT	1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2375763		A1	20021127	GB 2002-10225		20020503
	GB 2375763		B2	20030924			
	CA 2444940		AA	20030904	CA 2002-2444940		20020418
	WO 2003072565		A1	20030904	WO 2002-IB3832		20020418
			W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,			

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,  
 GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,  
 GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 BR 2002009194 A 20040608 BR 2002-9194 20020418  
 EP 1478635 A1 20041124 EP 2002-806883 20020418  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 GB 2387596 A1 20031022 GB 2003-15853 20020503  
 GB 2387596 B2 20040211  
 GB 2387844 A1 20031029 GB 2003-15852 20020503  
 ZA 2003008115 A 20040705 ZA 2003-8115 20031017  
 PRAI GB 2002-4607 A 20020227  
 WO 2002-IB3832 W 20020418  
 GB 2002-10225 A 20020503

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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GB 2375763	ICM	C07D307-87
GB 2375763	ECLA	C07D209/44; C07D307/87B
GB 2387596	ECLA	C07D307/87B
GB 2387844	ECLA	C07D209/44; C07D307/87B

GI



- AB A process for preparing highly pure salts of citalopram, such as I (R = CN; X = oxalate, hydrobromide, hydrochloride), for pharmaceutical compns. was described. Thus, citalopram contaminated with up to 5.0% of desmethyl citalopram was added to acetone and stirred for 15 min at 40° followed by addn of oxalic acid to form citalopram oxalate in 85% yield with desmethyl citalopram content <0.1%.
- ST citalopram salt prepn
- IT 59729-33-8P, **Citalopram** 207559-01-1P,  
**Citalopram** oxalate  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (process for the preparation of highly pure salts of **citalopram**)
- IT 85118-27-0P, **Citalopram** hydrochloride  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
 (process for the preparation of highly pure salts of **citalopram**)
- IT 59729-32-7P, **Citalopram** hydrobromide  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (process for the preparation of highly pure salts of **citalopram**)
- IT 67-64-1, Acetone, uses 108-20-3, Isopropyl ether 108-88-3, Toluene, uses 110-54-3, Hexane, uses 110-82-7, Cyclohexane, uses 142-82-5, Heptane, uses 1330-20-7, Xylene, uses

RL: NUU (Other use, unclassified); USES (Uses)  
 (process for the preparation of highly pure salts of citalopram)

IT 144-62-7, Oxalic acid, reactions 7647-01-0, Hydrochloric acid, reactions 7664-41-7, Ammonia, reactions 10035-10-6, Hydrobromic acid, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (process for the preparation of highly pure salts of citalopram)

IT 62498-67-3, Desmethyl citalopram 64169-39-7  
 64169-45-5 64372-56-1  
 RL: REM (Removal or disposal); PROC (Process)  
 (process for the preparation of highly pure salts of citalopram)

IT 59729-33-8P, Citalopram 207559-01-1P,  
 Citalopram oxalate  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (process for the preparation of highly pure salts of citalopram)

IT 85118-27-OP, Citalopram hydrochloride  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
 (process for the preparation of highly pure salts of citalopram)

IT 59729-32-7P, Citalopram hydrobromide  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (process for the preparation of highly pure salts of citalopram)

IT 62498-67-3, Desmethyl citalopram 64169-39-7  
 64169-45-5 64372-56-1  
 RL: REM (Removal or disposal); PROC (Process)  
 (process for the preparation of highly pure salts of citalopram)

L69 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2002:716262 HCAPLUS  
 DN 137:232543  
 ED Entered STN: 20 Sep 2002  
 TI Cyanation process for the preparation of citalopram  
 IN Biswas, Sujay; Sharma, Tarun Kant; Kumar, Yatendra; Sathyanarayana, Swargam; Vijayaraghavan, Bakthavathsalan  
 PA Ranbaxy Laboratories Limited, India  
 SO PCT Int. Appl., 14 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D307-77  
 ICS C07D307-81  
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45

FAN. CNT 1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002072565	A1	20020919	WO 2002-IB690	20020308
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2439856	AA	20020919	CA 2002-2439856	20020308
	EP 1370545	A1	20031217	EP 2002-702634	20020308
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2002007895	A	20041228	BR 2002-7895	20020308
	JP 2005500256	T2	20050106	JP 2002-571481	20020308
PRAI	IN 2001-DE264	A	20010309		
	WO 2002-IB690	W	20020308		

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002072565	ICM	C07D307-77	
	ICS	C07D307-81	
OS CASREACT 137:232543			
AB	An improved and industrially advantageous process for the preparation of citalopram and pharmaceutically acceptable acid addition salts consists of reacting a precursor substituted with a bromo or an iodo group in the same position as the cyano group in citalopram with a cyanide source in a solvent in the present of a N-containing base; the citalopram free base may then be salfied with a pharmaceutically acceptable acids.		
ST	citalopram prepn cyanation process		
IT	Amines, reactions RL: RGT (Reagent); RACT (Reactant or reagent) (bases; in the formation of complexes with cyanide sources for the cyanation of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane into citalopram)		
IT	Antidepressants (cyanation process for the preparation of citalopram)		
IT	Mental disorder (depression; cyanation process for the preparation of citalopram for the treatment of)		
IT	Cyanation (of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane with a complex of a cyanide source with a base)		
IT	Neutralization (of citalopram base with pharmaceutically acceptable acids)		
IT	62-53-3, Aniline, reactions 75-50-3, Trimethylamine, reactions 91-22-5, Quinoline, reactions 101-83-7, Dicyclohexylamine 108-18-9, <b>Disopropylamine</b> 108-48-5, 2,6-Lutidine 108-89-4, 4-Methylpyridine 110-86-1, Pyridine, reactions 121-44-8, Triethylamine, reactions 6674-22-2, DBU RL: RGT (Reagent); RACT (Reactant or reagent) (base; in the formation of complexes with cyanide sources for the cyanation of 1-(4'-fluorophenyl)-1-(3-dimethylaminopropyl)-5-iodo-or-bromophthalane into citalopram)		
IT	<b>59729-32-7P, Citalopram hydrobromide 59729-33-8P</b> , Citalopram RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (cyanation process for the preparation of citalopram)		
IT	7732-18-5, Water, uses 10035-10-6, Hydrogen bromide, uses RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses) (cyanation process for the preparation of citalopram HBr from)		
IT	<b>64169-39-7</b> 260066-78-2 RL: RCT (Reactant); RACT (Reactant or reagent) (cyanation process for the preparation of citalopram from)		
IT	143-33-9, Sodium cyanide 151-50-8, Potassium cyanide <b>544-92-3</b> , <b>Cuprous cyanide</b> 557-21-1, Zinc cyanide 12211-52-8, Ammonium cyanide RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent) (cyanation process for the preparation of citalopram from)		
IT	68-12-2, Dmf, uses 127-19-5, Dimethylacetamide 872-50-4, N-Methylpyrrolidone, uses 931-20-4, N-Methylpiperidone 1690-76-2 RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses) (solvent; cyanation process for the preparation of citalopram)		
RE. CNT 3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD		
RE.			
(1)	Bogeso; US 4136193 A 1979 HCPLUS		
(2)	Lundbeck, H; WO 0011926 A2 2000		
(3)	Lundbeck, H; WO 0013648 A2 2000 HCPLUS		
IT	<b>59729-32-7P, Citalopram hydrobromide 59729-33-8P</b> , Citalopram RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (cyanation process for the preparation of citalopram)		
IT	<b>64169-39-7</b>		

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram from)

IT 544-92-3, Cuprous cyanide  
 RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)  
 (cyanation process for the preparation of citalopram from)

L69 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2001:472398 HCPLUS  
 DN 135:61224  
 ED Entered STN: 29 Jun 2001  
 TI Method for the preparation and purification of citalopram  
 IN Villa, Marcos; Sbrogio, Federico; Dancer, Robert  
 PA H. Lundbeck A/S, Den.  
 SO PCT Int. Appl., 12 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 45

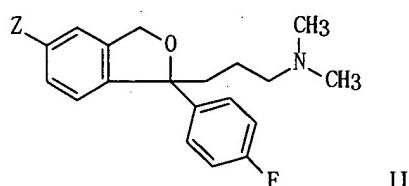
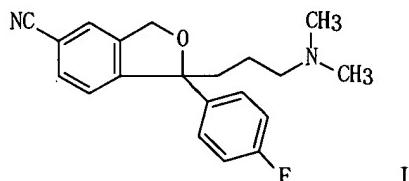
FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001045483	A2	20010628	WO 2001-DK147	20010307
	WO 2001045483	A3	20011227		
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	NL 1017525	C1	20010426	NL 2001-1017525	20010307
	CA 2360303	AA	20010628	CA 2001-2360303	20010307
	CA 2360303	C	20030812		
	EP 1181713	A2	20020227	EP 2001-913726	20010307
	EP 1181713	B1	20040929		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200201166	T1	20021021	TR 2002-200201166	20010307
	JP 2003517484	T2	20030527	JP 2001-546230	20010307
	BR 2001006272	A	20040615	BR 2001-6272	20010307
	EP 1462447	A2	20040929	EP 2004-4482	20010307
	EP 1462447	A3	20041117		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	AT 277920	E	20041015	AT 2001-913726	20010307
	DK 174018	B1	20020422	DK 2001-402	20010308
	GB 2357763	A1	20010704	GB 2001-5983	20010312
	GB 2357763	B2	20020116		
	GB 2359811	A1	20010905	GB 2001-15025	20010312
	GB 2359811	B2	20030305		
	CZ 292200	B6	20030813	CZ 2001-890	20010312
	FI 108639	B1	20020228	FI 2001-500	20010313
	NO 312462	B1	20020513	NO 2001-1271	20010313
	FR 2812877	A1	20020215	FR 2001-3455	20010314
	FR 2812877	B1	20030404		
	GR 1003874	B1	20020424	GR 2001-100132	20010316
	DE 10112829	C1	20020725	DE 2001-10112829	20010316
	CH 691535	A	20010815	CH 2001-545	20010322
	BE 1013212	A6	20011002	BE 2001-188	20010322
	NL 1018360	C1	20011004	NL 2001-1018360	20010622
	BE 1013213	A6	20011002	BE 2001-435	20010626
	CH 691998	A	20011231	CH 2001-1411	20010726
	ES 2170732	A1	20020801	ES 2001-1762	20010727
	AU 744112	B1	20020214	AU 2001-65477	20010827
	SE 517623	C2	20020625	SE 2001-3045	20010914
	SE 2001003045	A	20020623		

BG 106203	A	20020830	BG 2001-106203	20011210
ZA 2001010179	A	20021211	ZA 2001-10179	20011211
NZ 516298	A	20021220	NZ 2001-516298	20011220
HR 2002000004	A1	20030430	HR 2002-4	20020104
US 2002120005	A1	20020829	US 2002-46126	20020108
US 6455710	B2	20020924		
PRAI DK 2000-1929	A	20001222		
NL 2001-1017525	A	20001222		
EP 2001-913726	A3	20010307		
WO 2001-DK147	W	20010307		
GB 2001-5983	A3	20010312		
CH 2001-545	A	20010322		

CLASS	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 2001045483			
NL 1017525	ECLA	C07D307/87B	
EP 1462447	ECLA	C07D307/87B	
GB 2357763	ECLA	C07D307/87B	
GB 2359811	ECLA	C07D307/87B	
FR 2812877	ECLA	C07D307/87B	
DE 10112829	ECLA	C07D307/87B	
CH 691535	ECLA	C07D307/87B	
BE 1013212	ECLA	C07D307/87B	
NL 1018360	ECLA	C07D307/87B	
BE 1013213	ECLA	C07D307/87B	
CH 691998	ECLA	C07D307/87B	
US 2002120005	ECLA	C07D307/87B	
OS CASREACT 135:61224; MARPAT 135:61224			
GI			



AB A process for the preparation and purification of citalopram (I) is presented in which a benzoisofuran derivative [II; Z = iodo, bromo, chloro, CF<sub>3</sub>(CF<sub>2</sub>)<sub>n</sub>SO<sub>2</sub>O; n = 0-8] is subjected to a cyanide-exchange reaction with a cyanide source (e.g., cuprous cyanide). The resultant crude citalopram is optionally subjected to some initial purification and subsequently treated with an amide or an amide-like group forming agent (e.g., acetic anhydride), the reaction mixture is then subjected to an acid/base wash and/or crystallization and recrystn. of citalopram in order to remove the amides formed from the crude citalopram mixture, and the resulting citalopram product is optionally further purified, worked up and isolated as the base or a pharmaceutically acceptable salt.

ST citalopram prep'n purifn

IT Crystallization

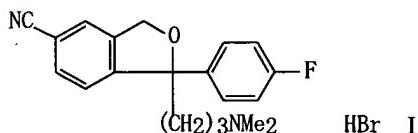
Recrystallization

Washing

(method for the preparation and purification of citalopram using)

- IT Acids, reactions  
Bases, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for the preparation and purification of citalopram using a washing with)
- IT Carbonitriding  
(method for the preparation of citalopram using)
- IT Amidation  
(method for the purification of citalopram using)
- IT Acid halides  
Anhydrides  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for the purification of citalopram using amide-forming)
- IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-50-8, Copper,  
uses 7440-66-6, Zinc, uses  
RL: CAT (Catalyst use); USES (Uses)  
(cyanidation catalyst for the preparation of citalopram)
- IT **59729-33-8P, Citalopram**  
RL: IMF (Industrial manufacture); PUR (Purification or recovery)  
; SPN (Synthetic preparation); PREP (Preparation)  
(method for the preparation and purification of **citalopram**)
- IT 64169-39-7 64169-45-5 260066-78-2 260066-82-8 345658-19-7  
345658-20-0 345658-21-1 345658-22-2 345658-23-3 345658-24-4  
345658-25-5 345658-26-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for the preparation of citalopram by the cyanidation of)
- IT 544-92-3, Cuprous cyanide 557-21-1, Zinc cyanide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for the preparation of citalopram using)
- IT 75-36-5, Acetyl chloride 108-24-7, Acetic anhydride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for the purification of crude citalopram by reaction of the crude  
reaction mixture with)
- IT **59729-33-8P, Citalopram**  
RL: IMF (Industrial manufacture); PUR (Purification or recovery)  
; SPN (Synthetic preparation); PREP (Preparation)  
(method for the preparation and purification of **citalopram**)

L69 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 1977:561413 HCPLUS  
 DN 87:161413  
 ED Entered STN: 12 May 1984  
 TI Quantitative structure-activity relationships in a series of selective  
5-HT uptake inhibitors  
 AU Bigler, Allan J.; Boegesoe, Klaus P.; Toft, Anders; Hansen, Villy  
 CS Dep. Synth. Chem., H. Lundbeck and Co. A/S, Copenhagen-Valby, Den.  
 SO European Journal of Medicinal Chemistry (1977), 12(3), 289-95  
 CODEN: EJMCA5; ISSN: 0223-5234  
 DT Journal  
 LA English  
 CC 1-3 (Pharmacodynamics)  
 Section cross-reference(s): 27  
 OS CASREACT 87:161413  
 GI



- AB Fifty-five 1-[3-(methylamino)propyl]- and 1-[3-(dimethylamino)propyl]-1-phenylphthalan derivs. were prepared and tested in vitro for inhibition of 5-hydroxytryptamine [50-67-9] uptake in blood platelets and in vivo for potentiation of 5-HT syndrome in mice. Quant. structure-activity relations were established, using the methods of Free-Wilson and Hansch.

Of several potent compds., Citalopram (I) [59729-33-8] was the most active.

- ST hydroxytryptamine inhibitor phthalan deriv
- IT Substituent effect  
(on (dimethylaminopropyl) phenylphthalan derivs. inhibition of hydroxytryptamine)
- IT Molecular structure-biological activity relationship  
(hydroxytryptamine-inhibiting, of (dimethylaminopropyl) phenylphthalans)
- IT Substituent constant  
( $\pi$ , of (dimethylaminopropyl) phenylphthalan derivs., lipophilicity in relation to)
- IT 109-54-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of, with benzophenone derivative)
- IT 74-96-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of, with phthalancarbonitrile derivative)
- IT 460-00-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of, with phthalide derivative)
- IT 789-96-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyanation of)
- IT 50-67-9, biological studies  
RL: BIOL (Biological study)  
(inhibition of, by (dimethylaminopropyl) phenylphthalans)
- IT 64372-57-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and Grignard reaction with bromobenzene derivative)
- IT 64372-58-3P 64372-61-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and Grignard reaction with propyl chloride derivs.)
- IT 64169-67-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and alkylation of)
- IT 64169-66-0P 64372-62-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyanation of)
- IT 64169-65-9P 64372-59-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)
- IT 64372-63-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)
- IT 10565-62-5P 10588-99-5P **59729-33-8P 62498-68-4P**  
62498-70-8P 64169-43-3P **64169-47-7P** 64169-54-6P  
64169-58-0P 64349-04-8P 64371-94-4P 64371-95-5P 64371-97-7P  
64371-98-8P 64371-99-9P 64372-01-6P 64372-02-7P 64372-03-8P  
64372-04-9P 64372-05-0P 64372-07-2P 64372-09-4P 64372-11-8P  
64372-13-0P 64372-14-1P 64372-15-2P 64372-16-3P 64372-18-5P  
64372-20-9P 64372-21-0P 64372-23-2P 64372-25-4P 64372-27-6P  
64372-28-7P 64372-29-8P 64372-31-2P 64372-32-3P 64372-34-5P  
64372-36-7P 64372-37-8P 64372-39-0P 64372-41-4P 64372-42-5P  
**64372-43-6P** 64372-44-7P 64372-45-8P 64372-47-0P  
64372-48-1P 64372-49-2P **64372-51-6P** 64372-53-8P  
64372-54-9P 64372-55-0P **64372-56-1P** 64406-38-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and hydroxytryptamine inhibition by)
- IT 64372-60-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)
- IT 64169-52-4P 64372-08-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 657-06-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of)

IT 64169-64-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of)

IT 59729-33-8P 62498-68-4P 64169-47-7P  
64372-43-6P 64372-51-6P 64372-56-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and hydroxytryptamine inhibition by)

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FILE 'HOME' ENTERED AT 15:49:51 ON 11 APR 2005

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